A COMBINATION OF DIRICHLET TO NEUMANN OPERATORS AND PERFECTLY MATCHED LAYERS AS BOUNDARY CONDITIONS FOR OPTICAL FINITE ELEMENT SIMULATIONS

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Abstract **– By combining Dirichlet to Neumann (DtN) operators and Perfectly Matched Layers (PML's) as boundary conditions on a rectangular domain on which the Helmholtz equation is solved, the disadvantages of both methods are greatly diminished. Due to the DtN operators, light may be accurately fluxed into the domain, while the PML's absorb light that is reflected from the corners of the domain when only DtN boundaries are used.**

I. Introduction

When performing simulations of optical phenomena, most existing methods calculate on a finite simulation window. The finiteness of the window should have as little influence on the calculations as possible; the boundaries must be treated such that they incorporate the effects of the exterior. They should be completely transparent for outgoing radiation, while allowing prescribed input fields to enter, taking into account any waveguides or other structure protruding through the boundaries.

This paper describes a finite element implementation of a Helmholtz equation solver on a finite, rectangular domain. Inside the domain, the refractive index may be arbitrary; outside, any structure is assumed to extend homogeneously into the exterior. This means that input and output waveguides may only run perpendicular to the boundaries.

To implement transparent boundary conditions, we combine the concepts of Dirichlet to Neumann operators, as described in e.g. [1, 2, 3], with Perfectly Matched Layers, as introduced by Berenger [4]. In the former method, the field on the boundary is expanded in modes on the exterior, where zero boundary conditions are employed to discretize the spectrum of modes, from which the operator is constructed that computes the normal derivative of the field for a given function of the field on the boundary. This normal derivative is chosen such that the flux of radiation on the boundary is purely outgoing. PML's are layers of artificial material, which are impedance-matched to the 'normal' material adjacent to them, but inside which the fields are strongly attenuated. They are often employed to absorb scattered radiation in e.g. FDTD methods.

Both these methods have their drawbacks. When using DtN operators on the boundary, the corners of the calculation window still act as scattering points. PML's don't have this problem, but for the Helmholtz equation, it is difficult to influx a prescribed field; since one can only easily prescribe the boundary conditions, an incoming field will first have to transfer through the PML. While it is possible to calculate the boundary condition that will correspond to a desired input field, it is not a trivial task and numerical errors can easily occur.

This paper first briefly describes the concepts of PML's and DtN operators in a finite element context, after which their combination is introduced. A numerical example shows that the approach allows strong scattering to leave the calculation window unobstructed.

II. Theory

A. Dirichlet to Neumann Operator

As in [2, 3], we perform finite element calculations on a rectangular calculation window, while we assume that the exterior behind each of the four boundary sections is uniform in the direction perpendicular to the boundary, and that the field on the lines extending perpendicularly from the edges of these sections equals zero. In fact, this means we calculate on a cross as shown in Figure 1.

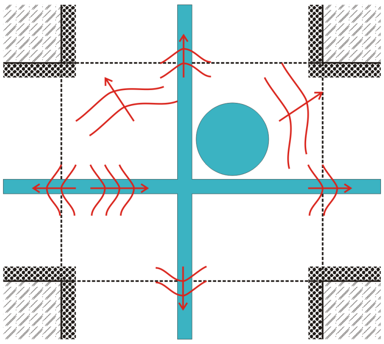

Fig. 1: A sample calculation window. The shaded regions at the corners are those regions where the field is zero. At all four boundaries, the the same type of DtN operator is used, which allows light to escape from the interior rectangle into the exterior wave-pipes. PML regions (dotted areas) of a certain thickness are added at the inward side of the wave-pipe borders, and on corresponding corner sections in the interior window.

When deriving a finite element approximation of the Helmholtz equation, the partial integration of the Laplace operator gives rise to the boundary term

$$\int_{\partial\Omega} v\partial_{\mathbf{n}}u \tag{1}$$

where v is a test function and u is the field on the boundary $\partial\Omega$ of the domain. For implementation into the finite element scheme, we need to express the normal derivative of u in terms of u itself, such that both can be connected smoothly to a purely outgoing exterior solution.

In the interior, the Helmholtz equation is discretized by means of a standard finite element scheme. In the exterior, contrary to [2, 3] where analytic modes are used, we also use (1D) finite elements to calculate the modes of the wave pipes; the locations of the nodes of the finite element mesh that lie on the boundary, and the shapes of their corresponding basis functions, are used to set up the finite element mode solver for the exterior. This gives a set of propagation constants β_m, where m runs from 1 to the number of internal nodes on the exterior, and finite element approximations of the corresponding modal fields.

The field on the boundary $u(y)$ can be decomposed into amplitudes of the 1D modes, using a projection operator $P_i(u)$:

$$a_m = P_m(u) = \int u(y)e_m(y)dy \tag{2}$$

where a_m is the amplitude of the mth mode and $e_m(y)$ is its field profile. Using this information, the DtN operator may be directly written down as:

$$D^+(u) = \partial_{\mathbf{n}}u = \sum_m -i\beta_m e_m(y)P_m(u) \tag{3}$$

Note that the sign in Eq. (3) is determined by the constraint of purely outgoing waves.

This DtN operator can be easily implemented into a finite element scheme.

At the corners of the domain the zero-field boundary condition causes reflections if light is scattered toward these corners. In [2] this scattering was decreased by moving the zero-field boundaries in the exterior away from the actual corners of the calculation window, but still some reflections remain.

B. *Perfectly Matched Layers*

Inside PML's, the Helmholtz equation gets modified into

$$\left(\sigma_y\partial_x\frac{1}{\sigma_x}\partial_x + \sigma_x\partial_y\frac{1}{\sigma_y}\partial_y + \sigma_x\sigma_y k_0^2 n^2\right)u = 0 \tag{4}$$

where σ_x and σ_y are $1 + is_x$ or $1 + is_y$, where s is a parameter that is proportional to the attenuation of the layer. We apply PML's to the structure as follows: In the exterior, a layer with constant nonzero s_x or s_y is added to the edges of the wave pipe, where the east and west exteriors get nonzero s_y and the north and south ones get nonzero s_x. Inside the domain, both s_x and s_y are made nonzero (and equal) only in rectangles near the corners; see Figure 1 for a graphical explanation.

When combining PML's with DtN operators, the modes and propagation constants of the outer regions, as well as the projection operators, are changed to accommodate for the nonzero s_x or s_y.

III. RESULTS

We show the effect of adding PML's to the simulations by comparing results on a strongly scattering structure, either with only DtN boundary conditions, or with combined DtN boundary conditions and PML's. Figure 2 shows the field of a particular, very strongly scattering, structure. It is clear that for this structure, the corners of the window cause a lot or extra scattering back into the window if only DtN operators are used. Adding the PML's cause the reflections from the corners to become so much smaller as to be invisible in the picture.

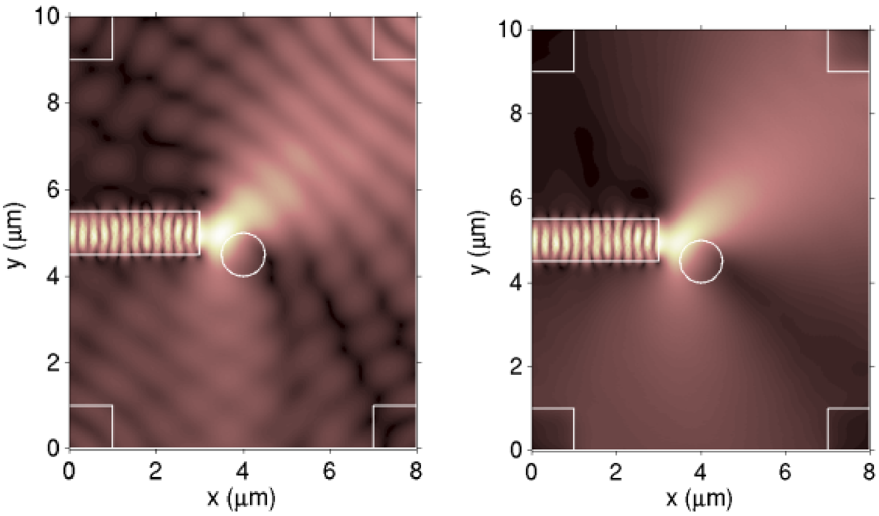

Fig. 2: Absolute value field plots of simulations with (right) and without (left) Perfectly Matched Layers. The fundamental mode of a silicon (n=3.4) waveguide in air (n=1.0) with a width of 1 μm comes in from the left; the waveguide ends abruptly after 3 μm, and there is a silicon disc with a radius of 0.5 μm located at position (4,4.5). In the right-hand picture, the 1 μm^2 squares at the corners have s_x and s_y of 0.4.

IV. CONCLUDING REMARKS

Adding Perfectly Matched Layers to the interior and exterior of a rectangular domain in which the Helmholtz equation is solved with Dirichlet to Neumann operators in the boundary conditions greatly decreases reflections from the corners of the domain. In principle, the concepts in this paper are extendible to fully 3D frequency-domain Maxwell equation simulations.

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